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Interplay of Kondo effect and superconducting gap in heavy fermion system

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Abstract : The heavy fermion system in superconducting state is described by the Hamiltonian containing the conduction electron term, on-site *f*-electron term besides the Kondo interaction and the Heisenberg interaction. The Hamiltonian is treated in mean-field approximation to find simultaneously the Kondo singlet term and antiferromagnetic correlation. The Kondo singlet parameter $\lambda = \left\langle f_{i,\sigma}^{\dagger} f_{i,\sigma} \right\rangle$ and *f*-electron correlation parameter $\Gamma = \left\langle f_{i,\sigma}^{\dagger} f_{j,\sigma} \right\rangle$ (nearest neighbours) are calculated by minimizing total energy of the system In addition to this, a BCS type phonon mediated Cooper pairing is considered to find the superconducting gap equation. In this communication, interplay of Kondo effect and superconducting gap of the heavy fermion system is studied through the self-consistent solution of these two parameters.

Keywords : Heavy fermions, Kondo effect, heavy fermion superconductivity.

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1. Introduction

The ground state of Kondo atom is a non-magnetic singlet state in case of a single impurity [1], while there is a strong competition between the Kondo effect and the magnetic ordering in the heavy fermion compounds [2]. Thus cerium (Ce) Kondo compounds are; at low temperatures, either non-magnetic as in case of single impurity or magnetically ordered [3,4]. The well known 'Doniach diagram' gives a qualitative description of the competition between the Kondo effect and the magnetic ordering as a function of the exchange integral J_K (with $J_K < 0$). Kondo temperature T_K increases experimentally with $|J_K|$ while the real magnetic ordering temperature T_N increases initially with increasing $|J_K|$, then passes through a maximum and tends to zero at a critical value. Such behaviour of T_N has been observed experimentally in $CePd_2Al_3$, $CeAl_2$, $CePd_2Si_2$ and $CeRb_2Si_2$ [5]. Such a description of Doniach appears to be too simplified for the really observed Kondo temperature T_K. Iglesias and coworkers [6,7] have taken the effect of antiferromagnetic correlation in the non-magnetic phase. Moreover the occurrence of short range magnetic correlation has been observed experimentally by neutron diffraction experiment at low temperatures in $CeCu_6$, $CeRu_2Si_2$ [8,9]. It has been found that incommensurate and antiferromagnetic correlations develop at low temperatures below $T_N \simeq$ 60 – 70 K in $CeRu_2Si_2$ [8,9] or $T_N \simeq 10$ K in $CeCu_6$ [8], which are clearly larger than Kondo temperature $T_K \simeq 14$ – 23 K in $CeRu_2Si_2$ or T_K ~5 K in $CeCu_6$. Recently, Rout *et al* have studied the superconducting gap of heavy fermions superconductivity through periodic Andersen Model wherein Kondo singlet is taken as a parameter only, but the Coulomb correlation is considered in Hartree-fock type mean-field approximation [10].

In the present communication, we propose a model for heavy fermion superconductors to describe the Kondo correlations observed in Kondo lattice systems. The formalism and the expression for short range magnetic

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corelation (Γ) and Kondo correlation (λ) are described in Section 2. A BCS type mean field Hamiltonian is considered for the superconductivity in heavy fermion systems. The mean-field parameters are calculated in Section 3. Finally, the results are discussed in Section 4.

2. Formalism

We consider the following to discribe the Kondo lattice with short-range magnetic correlation in normal phase, as described by Iglesias *et al* [6]

$$\mathcal{H} = \sum_{k,\sigma} \epsilon_k c^\dagger_{k,\sigma} c_{k,\sigma} + E_0 \sum f^\dagger_{i,\sigma} f_{i,\sigma}$$

$$- J_H \sum_{i,j} S^f_i . S^f_j - J_K \sum c^f_i . S^f_i \tag{1}$$

where $c_{k,\sigma}, f_{i,\sigma}, s^c_i, S^f_i$ are, respectively, the annihilation operator of conduction electrons for wave vector $\boldsymbol{k}$ and spin σ, the annihilation operator of f-electrons at site i and spin σ, the spin operator for conduction and f-electrons. In eq. (1), we take a zero width f-band E_0, a conduction band of width $2W$ and a constant density of states. The third term describes the Heisenberg interaction between neighouring f-magnetic moments. Here $J_H > 0$ for a ferromagnetic coupling and $J_H < 0$ for an antiferromagnetic coupling. The last term is the conduction and f-electron exchange term and J_K (< 0) is Kondo coupling. We treat the Hamiltonian in eq. (1) in a 'mean-field' approximation to find simultaneously the Kondo effect and the antiferromagnetic correlations. The two mean-field parameters are (i) $\lambda = < f^\dagger_{i,\sigma} c_{i,\sigma} >$ which describes the formation of Kondo singlet and (ii) $\Gamma = < f^\dagger_{i,\sigma} f_{j,\sigma} >$ (for nearest neighbours) which accounts for magnetic correlation between neighbouring localised spins. Within the mean-field approximation Hamiltonian in eq. (1) can be written after Fourier transformation as :

$$\mathcal{H}_0 = \sum_{k,\sigma} \epsilon_k c^\dagger_{k,\sigma} c_{k,\sigma} + \sum_{k,\sigma} \epsilon_f (k) f^\dagger_{k,\sigma} f_{k,\sigma}$$

$$+ V \sum_{k,\sigma} \left(c^\dagger_{k,\sigma} f_{k,\sigma} + f^\dagger_{k,\sigma} c_{k,\sigma} \right)$$

$$- 2J_K \lambda^2 - Z_1 J_H \Gamma^2, \tag{2}$$

where $\epsilon_f(k) = E_0 + B \epsilon_k$, with $B = \dfrac{Z_1 J_H \Gamma}{W}$, W = half band width and $V = J_K \lambda$ with the nearest neighbour sites Z_1.

The mean field Hamiltonian $\mathcal{H}_I$ describes the superconductivity in the heavy fermion systems through the BCS type Cooper pairing mechanism.

$$\mathcal{H}_I = -\Delta \sum \left(c^\dagger_{k,\uparrow} c^\dagger_{-k,\downarrow} + c_{-k,\downarrow} c_{k,\uparrow} \right) \tag{3}$$

where Δ is the momentum independent superconducting gap parameter.

3. Calculation of mean-field parameters

The four coupled one-electron Green's functions are defined as

$$G_1(k,\omega) = \left\langle\left\langle c_{k,\uparrow} ; c^\dagger_{k,\uparrow} \right\rangle\right\rangle_\omega ,$$

$$G_2(k,\omega) = \left\langle\left\langle c_{-k,\downarrow} ; c^\dagger_{k,\uparrow} \right.\right.$$

$$G_3(k,\omega) = \left\langle\left\langle f_{k,\uparrow} ; c^\dagger_{k,\uparrow} \right.\right.$$

$$G_4(k,\omega) = \left\langle\left\langle f_{-k,\downarrow} ; c^\dagger_{k,\uparrow} \right.\right. \tag{4}$$

These Green's functions are calculated by equations of motions of Zubarev technique [11] and the Green's functions $G_1(k,\omega)$ and $G_2(k,\omega)$ are expressed in closed form as given below :

$$G_1(k,\omega) = \frac{1}{2\pi |D(\omega)|} \left[\left(\omega^2 - \epsilon^2_f (k)\right)\left(\omega + \epsilon_k\right) - V^2 \left(\omega - \epsilon_k\right) \right], \tag{5}$$

$$G_2(k,\omega) = \frac{-\Delta}{2\pi |D(\omega)|} \left(\omega^2 - \epsilon^2_f (k)\right), \tag{6}$$

where

$$|D(\omega)| = \omega^4 - S_1 \omega^2 + T_1 \tag{7}$$

with

$$S_1 = E^2_k + \epsilon^2_f (k) + 2V^2 , \tag{8}$$

$$T_1 = E^2_k \epsilon^2_f (k) - 2\epsilon_k \epsilon_f (k) V^2 + V^4 , \tag{9}$$

$$E^2_k = \epsilon^2_f (k) + \Delta^2 . \tag{10}$$

The poles of the Green's functins $G_1(k,\omega)$ and $G_2(k,\omega)$ give four quasi-particle bands $\pm$ w_j (j = 1, 2). The quasi particle bands are given by

$$\omega_1 = \pm \left(\frac{S_1 + \sqrt{S^2_1 - 4T_1}}{2} \right)^{\frac{1}{2}} \tag{11}$$

$$\omega_2 = \pm\left(\frac{S_1 - \sqrt{S_1^2 - 4T_1}}{2}\right)^{\frac{1}{2}} \tag{12}$$

The four qausi-particle bands are strongly influenced by the model parameters of sub-atomic systems of the heavy fermion superconductors.

The momentum independent super conducting gap Δ is defined as

$$\Delta = V_0 \sum \left\langle c^{\dagger}_{k,\uparrow} c^{\dagger}_{-k,\downarrow} \right\rangle, \tag{13}$$

where V_0 is the effective attractive interaction between the electrons. Although the HFS are unconventional superconductors, one can observe some important features from the Hamiltonians with pairing within weak coupling. BCS approach for which the relation $T_c << w_D$ (Debye frequency) must hold. The superconducting gap is found to be

$$\Delta = g\int_{-w_D}^{w_D} d\in_k \frac{-}{2\left(\omega_1^2 - \omega_2^2\right)}\left[F_1(k,T) - F_2(k,T)\right], \tag{14}$$

where

$$F_1(k,T) = \frac{\omega_1^2 - \in_f^2(k)}{\omega_1^2}\tanh\left(\frac{\beta\omega_1}{2}\right), \tag{15}$$

$$F_2(k,T) = \frac{\omega_2^2 - \in_f^2(k)}{\omega_2^2}\tanh\left(\frac{\beta\omega_2}{2}\right) \tag{16}$$

Here, $\sum_k$ is replaced by $\int N(0)d\in_k$, with integration limit $-w_D$ to w_D, where $N(0)$ is the density of states of the conduction electrons at the Fermi level and $g = N(0)V_0$.

Thus within the mean-field approach, the two hybridized quasi-particle bands are ω_1 and ω_2, as given in eq. (11) and eq. (12). The total energy of the HF superconducting system is

$$E = 2\sum_k \left[\omega_1 f(\beta\omega_1) - \omega_1 f(-\beta\omega_1) + \omega_2 f(\beta\omega_2) - \omega_2 f(-\beta\omega_2)\right] - Z_1 J_H \Gamma^2 - 2J_K\lambda^2 - |\Delta|, \tag{17}$$

where the summation is made over all the k-states and the $f(\beta\omega)$ reperesnts the Fermi-Dirac distribution function with $\beta = \frac{1}{K_B T}$. The temperature-dependent mean-field parameter $\lambda(T)$ represnting the Kondo singlet formation is determined by minimizing the total energy given in eq. (17) with respect to $\lambda(T)\left(i.e. \frac{\partial E}{\partial \lambda} = 0\right)$ which gives the expression for $\lambda(T)$ as

$$\lambda(T) = \sum \left| \frac{V}{\omega_1} F_3(k,T) - \frac{V}{\omega_2} F_4(k,T) \right. \tag{18}$$

where

$$F_3(k,T) = \frac{\omega_1^2 - V^2 + \in_k \in_f(k)}{\sqrt{S_1^2 - 4T_1}}$$

$$\tanh\left(\frac{\beta\omega_1}{2}\right) \quad \frac{\beta\omega_1}{2\cosh^2\left(\frac{\beta\omega_1}{2}\right)} \tag{19}$$

$$F_4(k,T) = \frac{\omega_2^2 - V^2 + \in_k \in_f(k)}{\sqrt{S_1^2 - 4T_1}}$$

$$\tanh\left(\frac{\beta\omega_2}{2}\right) + \frac{\beta\omega_2}{2\cosh^2\left(\frac{\beta\omega_2}{2}\right)} \tag{20}$$

Similarly, the minimization of the total energy $i.e. \frac{\partial E}{\partial \Gamma} = 0$ gives the expression for the f-electron correlation.

To study the Kondo effect on the superconducting gap, the different model parameters are scaled with respect to the Debye frequency w_D.

$$z = \frac{\Delta}{w_D},\ d = \frac{E_0}{w_D},\ g_1 = \frac{J_K}{w_D},\ g_2 = \frac{J_H}{w_D}$$

$$t = \frac{K_B T}{w_D},\ B = \frac{Z_1 g_2 \Gamma}{p},\ p = \frac{W}{w_D},\ \upsilon = g_1\lambda.$$

4. Results and discussion

The different parameters describing the Kondo effect and superconducting (SC) gap in HFS are the bare f-level position d, magnetic correlation coupling parameter g_2, Kondo coupling parameter g_1, effective hybridization parameter λ super conducting gap parameter z, superconducting coupling constant g and reduced temperature t. The above parameters influence the SC gap parameter z of HFS and effective hybridisation parameter λ. We evaluate parameter z and λ by self consistent method and neglect the effect of magnetic correlation in this communication. We set the Fermi level $\epsilon_F = 0$ under the half-filling situation.

Before studying the interplay of the superconductivity and Kondo effect, we plot the temperature dependence of the superconducting (SC) gap z and the Kondo singlet(KS) parameter λ as shown in Figure 1. The SC shows BCS

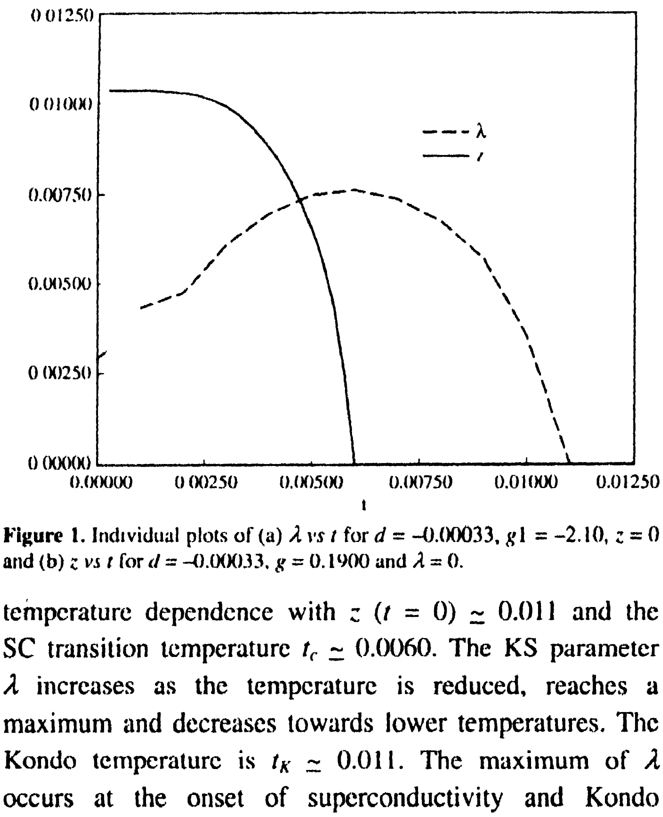

Figure 1. Individual plots of (a) λ vs t for $d = -0.00033$, $g1 = -2.10$, $z = 0$ and (b) z vs t for $d = -0.00033$, $g = 0.1900$ and $\lambda = 0$.

temperature dependence with z (t = 0) $\simeq$ 0.011 and the SC transition temperature $t_c \simeq$ 0.0060. The KS parameter λ increases as the temperature is reduced, reaches a maximum and decreases towards lower temperatures. The Kondo temperature is $t_K \simeq$ 0.011. The maximum of λ occurs at the onset of superconductivity and Kondo singlet formation is reduced inside the superconducting phase.

For the interplay of superconductivity and Kondo singlet formation, the temperature dependence of the SC gap z and KS parameter A is shown in Figure 2. The SC gap z (t = 0) is supressed a small amount, while the λ (t = 0) is supressed considerably. Moreover, the maximum of λ occurs at the on-set of superconductivity at t_c and is gradually suppressed in the superconductivity phase during the interplay. It is observed that the SC transition temperature ($t_c \simeq$ 0.0045) and Kondo temperature ($t_K \simeq$ 0.006) are reduced considerable compared to their individual values (Figure 1). The SC coupling parametr ($g \simeq$ 0.190) and Kondo coupling parameter $g1 \simeq -2.10$ satisfy the experimental situation *i.e.* $t_K > t_c$ for the heavy fermion systems : $CeCu_6$ [8] and $CeRu_2Si_2$ [8,9].

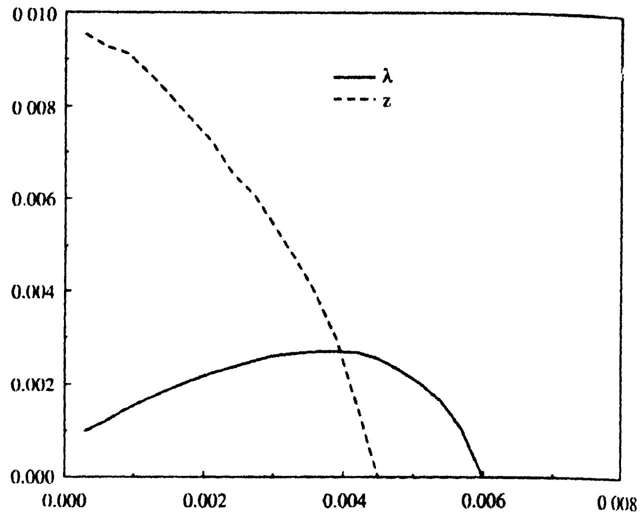

Figure 2. Self-consistent plots of λ vs. t and z vs. t for the same set of parameters $d = -0.00033$, $g1 = -2.10$, $g = 0.1900$ as shown in Figure 1.

The effect of the SC coupling g on the SC gap z and KS parameter λ is shown in Figure 3. The SC coupling has little effect on λ in the SC phase. However, it enhances λ in normal phase for temperature $t > t_c$ and

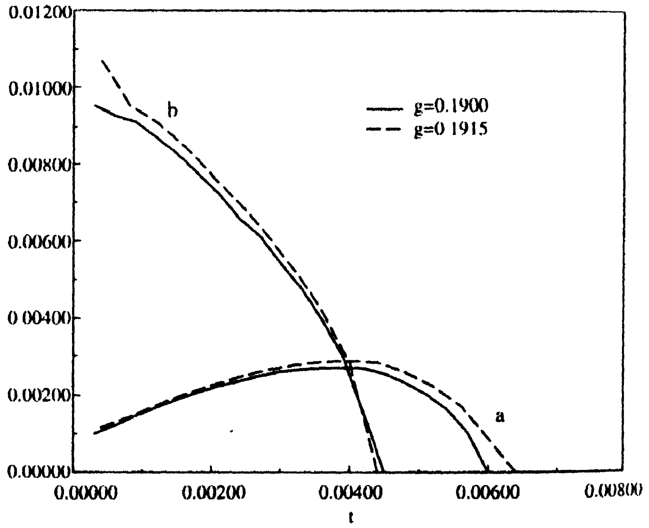

Figure 3. Plots of (a) λ vs t and (b) z vs t for the parameters $d = -0.00033$, $g1 = -2.10$ and for different g = 0.1900, 0.1915.

results the enhancement of Kondo temperature t_K. The SC gap z is enhanced with the increase of the SC coupling as predicted by BCS theroy for temperature $t < t_c$; but the SC transition temperature t_c is supressed due to the interplay. It so happens because $\left\langle c^{\dagger}_{k,\sigma} f_{k,\sigma} \right\rangle$ amplitude is enhanced resulting in the breaking down of the SC amplitude $\left\langle c^{\dagger}_{k,\uparrow} c^{\dagger}_{-k,\downarrow} \right\rangle$ near the SC transition temperature t_c and below.

The effect of Kondo coupling $g1$ on the SC gap z and the parameter λ is shown in Figure 4. The Kondo

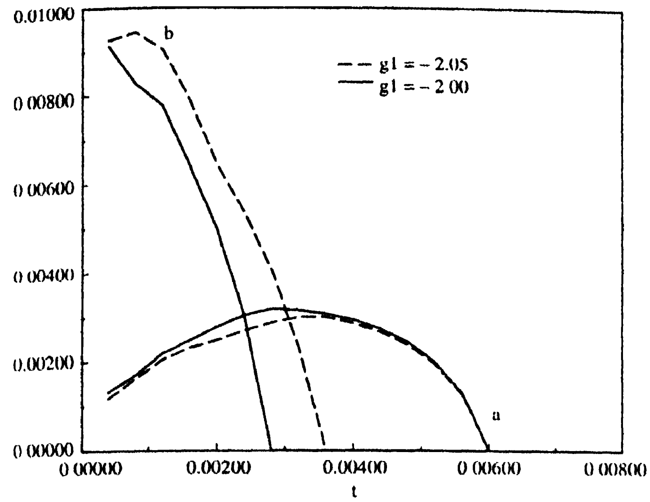

Figure 4. Plots of (a) λ *vs* t and (b) z *vs* t for the parameters $d = -0.00033$, $g = 0.1910$ and for different $g1 = -2.05, -2.00$.

coupling $g1$ does not change the Kondo temperature t_K and parametr λ for temperature $t > t_c$, but supresses the Kondo singlet formation in the SC phase for $t < t_c$. The Kondo coupling $g1$ enhances both the SC gap through out the temperature ranges as well as the SC transition temperature.

The influence of the position of f-level on SC gap z and the parameter λ is shown in Figure 5. Here negative

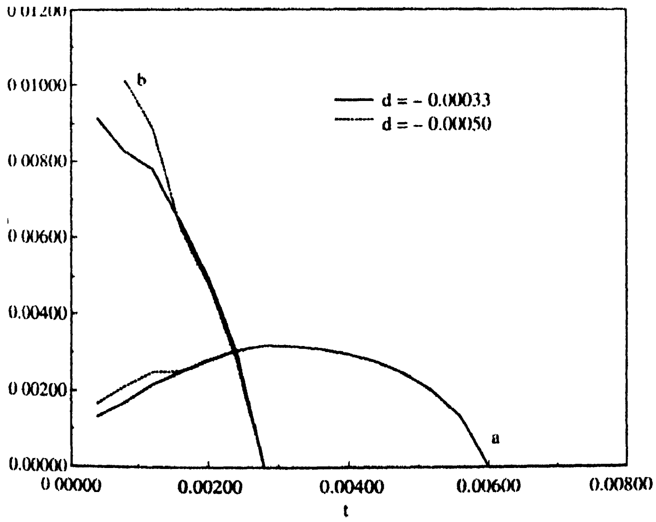

Figure 5. Plots of (a) λ *vs* t and (b) z *vs* t for the parameters $g = 0.190$, $g1 = -2.00$ and for different $d = -0.00033, -0.00050$.

d means the f-level lies below the Fermi level from $d = -0.00033$ to $d = -0.00050$, the SC transition temperature as well as the Kondo temperature t_K are unaffected. However, the SC gap z and Kondo singlet formations are enhanced at lower temperature, as the f-level moves down the Fermi level. In this mean-field approach, the large variation of f-level position destabilizes the co-existence phase.

5. Conclusion

The Kondo lattice model including •nearest neighbour magnetic exchange interaction is studied here in a mean-field approximation describing both the Kondo state and the intersite magnetic correlation. The BCS mean-field approximation is considered to study the superconductivity in HFS. The SC gap z and Kondo singlet parameter λ are solved self consistently and the effect of the model parameters on them is discussed. The interplay of gap z and parameter λ leads to the suppression of the both as well as the t_c and t_K. The SC coupling enhances the t_K and suppresses the t_c slightly and enhances the SC gap as expected by BCS theory. The Kondo coupling $g1$ enhances the SC gap z as well as the SC transition temperature t_c, while keeping the Kondo temperature t_K unaffected. The effect of short range magnetic correlation is not considered here. It may have a great bearing on the SC gap and Kondo singlet formation and the co-existence phase.

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References

[1] K G Wilson *Rev. Mod. Phys.* **47** 773 (1975)

[2] S Doniach *Phys. Rev.* **B91** 321 (1977)

[3] J G Sereni in *Handbook on the Physics and Chemistry of Rare-Earth* (eds) K A Gschnddner (Jr) and L Eyring **Vol. 15** p1 (Amsterdam : Elsevier) (1999)

[4] B Coqblin, J Arispe, J R Iglesias, C Lacroix and Karyn Le Hur *J. Phys. Soc. Jpn.* **65** (1996) Suppl-B 64 and references therein

[5] R Movshovich, J Graf, D Mandrus, M F Hundley, J D Thompson, R A Flschet, N E Phillips and J L Smith *Proc. SCES'95 Conf (Goa, India) Physica* **B223-224** 126 (1995)

[6] J R Iglesias, C Lacroix and B Coqblin *Phys. Rev.* **B56** 11820 (1997)

[7] C Lacroix, J R Iglesias, J Arispe and B Coqblin *Physica* **B230-232** 503 (1997)

[8] J Rossat-Mignod, L P Regnualt, J L Jacond, C Vettier, P Lejay, J Flouquet, E Walker, D Jaccard and A Amato *J. Magn. Magn. Mater.* **76-77** 376 (1988)

[9] L P Regnault, W A C Erkelens, J Rossat, -Mignod, P Lejay and J Flouquet *Phys. Rev.* **B38** 4481 (1988)

[10] G C Rout and S Das *Physica* **C339** 17 (2000)

[11] D N Zubarev *Sov. Phys. UPS* **95** 17 (1960)